Promoting Representational Competence with Molecular Models in Organic Chemistry

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ABSTRACT: Mastering the many different diagrammatic representations of molecules used in organic chemistry is challenging for students. This article summarizes recent research showing that manipulating 3-D molecular models can facilitate the understanding and use of these representations. Results indicate that students are more successful in translating between diagrams when they have models available, that using a model to enact the translation process in the world is predictive of learning, and that using models as feedback (to check the accuracy of diagram translation) is particularly effective. Model-based feedback is superior to verbal feedback alone, models scaffold learning rather than act as a crutch, learning with model-based instruction is resilient over a delay of several days, and learning with models transfers to performance when models are no longer available. Finally, virtual models are equivalent to hand-held models in promoting learning in the studied contexts.

KEYWORDS: *Second-Year Undergraduate, Curriculum, Organic Chemistry, Computer-Based Learning, Manipulatives, Molecular Modeling*
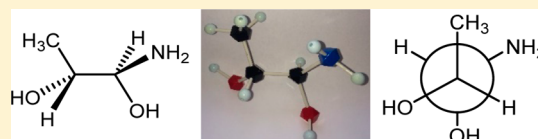
Visual-spatial representations, including various types of diagrams of molecules, are essential for communication, research, and teaching in chemistry.[1] Learning the conventions and uses of these representations is a crucial aspect of chemistry education,[2] which is sometimes referred to as acquiring *representational competence*.[3] However, mastering disciplinary representations is often challenging for students.[4,5] This article summarizes recent work investigating methods of facilitating the development of representational skills in organic chemistry through the use of 3-D molecular models.[6−8]

Organic chemists use a wide range of representations of molecules both in the laboratory and in the classroom. These include verbal representations, equations, 2-D spatial representations (diagrams), such as Lewis structures, line (skeletal) structures, Fischer and Newman projections, and 3-D models, which can be hand-held or virtual (computer-based). Molecular models are often used in organic chemistry lectures, and can support learning in this domain.[9−13] Instructors regularly urge students to use models to help them learn; however, a recent survey of chemistry students revealed that they rarely use models, even when encouraged to do so by their instructor.[14] Moreover, there are few well-controlled empirical studies that document how to best use molecular models in teaching and learning.

Here, we focus on ways of fostering students' skills in drawing, interpreting, and translating between spatial representations, that is, diagrams and 3-D models. Developing these skills is essential for students in chemistry.[3,6,15] Specifically, students must learn to interpret the spatial form implied by structural representations so that they can understand the relationship between a molecule's structure and its chemical reactivity.[16,17] However, spatial representations are not always easy to master.[18,19] Specifically, beginning students have difficulty translating between different representations of the same molecule,[3,5,20] and this is particularly true of students with low spatial ability.[18]

In terms of theories of human cognition, learning to use multiple spatial representations induces high cognitive load, that is, it places a demand on our limited spatial working memory.[21] First, molecules made up of several atoms in specific spatial configurations are quite complex, so that mental representations of these entities are likely to overload limited cognitive capacities. Second, interpreting different diagrams involves recalling and imagining how different diagrammatic conventions depict 3-D spatial entities in the two dimensions of the printed page.[22] Third, translating between different diagrams involves mentally transforming these representations (e.g., rotating a molecule from the perspective shown in a dash-wedge diagram to the view shown in a Newman projection).

BENEFITS OF USING 3-D MOLECULAR MODELS

We propose three ways in which manipulating 3-D molecular models can help students develop representational competence in organic chemistry. First, manipulating models enables students to *off-load cognition*. Second, the use of *multiple representations* helps students build more complete mental models. Third, 3-D models help students integrate new information with their preexisting knowledge (*elaborative*

encoding) by offering multiple perceptual modalities to support encoding and recall of the represented molecules.

Off-Loading Cognition

Manipulating molecular models can help students learn new diagrams by off-loading cognition onto external objects and performed actions rather than those imagined.[23] This, in turn, reduces the demand on working memory and lowers a student's cognitive load.[24] First, a molecular model represents a molecule externally so that students do not need to imagine and maintain a 3-D representation in working memory.[25] Second, the 3-D relations between atoms in a molecule are directly visible in a 3-D model (in contrast with diagrams, in which understanding the 3-D relations depends on conventions).[26] Third, one can more easily manipulate and observe the results of manipulations of an external representation than one can transform as an internal representation.[27] With the resulting decrease in cognitive load, students should be able to invest more cognitive effort in mapping conventions and translating between different representations, leading to improved learning.[5]

Multiple Representations

Research in the cognitive and learning sciences has found that students develop more complete and coherent mental models of concepts when these concepts are learned from multiple representations.[28] Different representations of molecules make salient different aspects of the molecular structure; each representation offers a unique perspective of a represented molecule's structure although no single representation, including molecular models, depicts a molecule perfectly. For example, although a perspective diagram (dash-wedge) and Newman perspective can depict the same molecule, a more complete understanding of the underlying molecule is achieved with multiple representations. Understanding which β-hydrogen is eliminated in an E2 reaction might be difficult with a perspective diagram but is relatively straightforward with a Newman Projection. With multiple representations, students should be able to build more complete mental models of the targeted entities and concepts, leading to improved organization and integration into memory.

Elaborative Encoding

Manipulating 3-D models can also support how new information is stored in memory by allowing for what cognitive psychologists refer to as *elaborative encoding*. Physical enactment, that is, learning by doing[29−31] and perception of nonvisual information[32] can enhance storage and retrieval of information in long-term memory. Nonvisual sensory cues from touch and proprioception (sensing of self-motion) can give students a richer experience that can lead to better memory storage and recall.[33,34] As an example, virtual models have been shown to be helpful by highlighting, through touch, the contribution of repulsive forces between molecules during a chemical reaction.[35] With more elaborate encoding, students should be able to better store and recall information from memory because they have multiple retrieval cues.

In sum, 3-D molecular models enable students to perceive 3-D spatial relations between parts of a molecule and add additional representations and perceptual modalities leading to richer memories. We suggest that models offer learning benefits because molecules and chemical reactions are rendered for visual inspection thereby reducing demand on spatial working memory, allowing cognitive effort to be better invested in meaningful learning. The studies we review here were motivated by the hypothesis that physically manipulating models benefits the mastery of more abstract 2-D diagrams.

■ LEARNING WITH 3-D MODELS IN CHEMISTRY

Here, we describe a series of studies in which cognitive psychologists collaborated with organic chemistry instructors to examine the benefits of models in teaching students about the conventions of different molecular diagrams and how to translate between these representations. First, Stull, Hegarty, Dixon, and Stieff[8] conducted three studies to investigate if and how students spontaneously used models to support their reasoning when translating between different structural diagrams, and what methods increased students' productive use of models. Following on these results, Padalkar and Hegarty[6] conducted two studies to develop and test a model-based feedback intervention to encourage model use and improve performance when translating structural diagrams. Extending both efforts, in two studies, Stull and Hegarty[7] tested whether model-based feedback also contributed to long-term learning and compared model-based feedback from hand-held and virtual models.

Participants were undergraduate students at a research university who were either concurrently or previously enrolled in an organic chemistry course. Participants were tested individually. After giving informed consent, they studied a diagram description to refresh their understanding of the three common molecular diagrams (see Figure 1a−c): Fischer
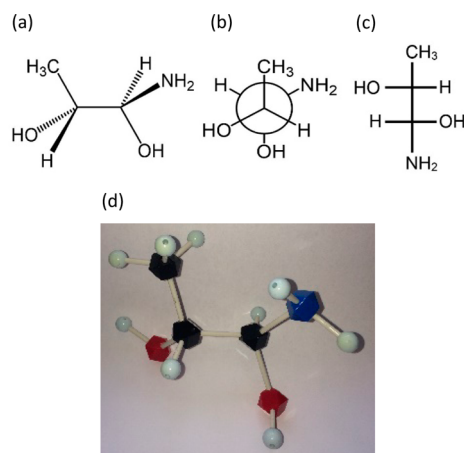
Figure 1. Four molecular representations: (a) dash-wedge diagram, (b) Newman projection, (c) Fischer projection, and (d) a hand-held (ball-and-stick) model.

projections, Newman projections, and dash-wedge diagrams of common organic chemistry molecules having three-, four-, and five-carbon backbones. For the task, students were given one diagram and asked to draw the same molecule but in a different diagrammatic form. For example, they might be given a Newman projection of a molecule and asked to draw the Fischer projection of the same molecule. After the translation trials, participants completed a short demographic questionnaire followed by a spatial ability test.[36] Data analyzed included accuracy of the diagrams drawn and a tally of the actions employed when using the models to solve problems.

Spontaneous Use of Molecular Models

As a first step, Stull, Hegarty, Dixon, and Stieff[8] conducted a correlational study (Study 1) to examine if organic chemistry

students spontaneously used hand-held molecular models while translating between diagrams, and if so, how model use correlated with accuracy in diagram translation. On each translation trial, a hand-held model of the molecule in question was placed on the table in front of and within easy reach of the participants, who were neither encouraged nor hindered from viewing or moving the models. Would students enact the translation using the model provided? Would they use the models to check their completed translations? The main hypothesis was that use of models to off-load cognition would be associated with translation accuracy. Specifically, aligning the model to the orientation of the diagram to be drawn should be a predictor of how well students are able to translate between different structural diagrams. Videotapes were coded for three main ways in which students used the models: moving the model to align it in the general orientation of the starting diagram (Align-Start), reconfiguring the model (Reconfigure) by rotating the substituents around their bonds and rotating the model to align it with the general orientation of the target diagram (Align-Target). A second hypothesis was that spatial ability would be associated with translation accuracy in general because the task of encoding and translating between structural diagrams is highly demanding of spatial working memory, which are related to spatial ability.[21]

As shown in Figure 2, performance on this task was relatively poor in Study 1 ($n = 30$). An important result was that, as
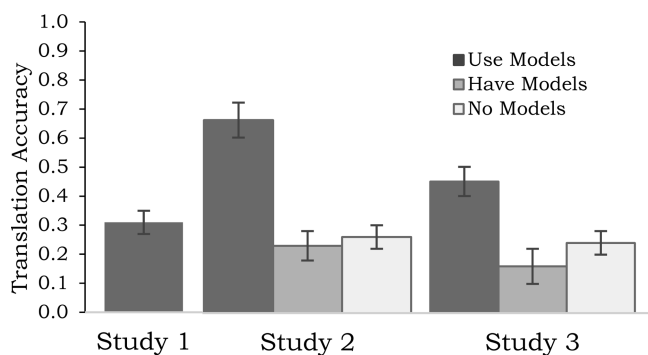
Figure 2. Means for translation accuracy for Studies 1, 2, and 3 from Stull et al.[8] Translation accuracy is reported as proportion correct on diagram translations. Sample sizes were 30 for Study 1, 64 for Study 2, and 59 for Study 3. Error bars show standard error of the mean.

predicted, there was a positive correlation between use of the models and translation accuracy. The most common type of model interaction, and the one most highly correlated with accuracy ($r = 0.52$, $p < 0.01$), was to rotate the model to the orientation of the intended diagram (Align-Target), as one might expect if participants performed an external action that replaced or augmented a mental process (e.g., mental rotation). Importantly, aligning the model with the target diagram typically occurred before or during the drawing of the target and rarely occurred after the diagram was complete, suggesting that it was part of the solution process and not just a check of their answer.

A second result of this study was that, in spite of the benefit of models, about half (53%) of the participants did not use the model on any of the trials and only one participant used a model on every trial. It is possible that students did not understand the correspondence between parts of the diagram and parts of the model, that students did not realize how the

models could be used to help with the translations, or that students preferred to use analytic translation strategies.

In addition, as predicted, translation accuracy was positively correlated with spatial ability ($r = 0.58$, $p < 0.01$). Statistical analyses revealed that using a model to enact the translation, such as aligning the model to the diagram to be drawn, and spatial ability were significant and independent predictors of translation accuracy.

The results of this first study raised two important questions. Why were students not using models to help them solve the diagram translation problems and how could students be encouraged to use models to help them develop their representational competence?

Encouraged Use of Models

Study 2 examined whether providing and encouraging students to use models offers an advantage over not receiving models.[8] Students were alternatively assigned to one of two conditions, those who received models (Models group) or those who received no models (Control group). For the Models group, a hand-held model of the molecule in question was placed on the table in front of and within easy reach of the participant and students in this group were given written explicit instructions and oral encouragement to use the models. The predictions were that with this explicit encouragement, students in the models groups would use models more and translate diagrams more accurately than students in the Control group. In addition, it was predicted that model use and spatial ability would independently predict translation accuracy.

As predicted, the Models group ($n = 32$) significantly outperformed ($d = 0.56$) the Control group ($n = 32$) on accuracy in translating between diagrams (see Figure 2). However, some participates still ignored the models, even with explicit encouragement. Moreover, when the Models group was split in two subgroups ["Use Models" group (participants who aligned the model to the target diagram on 50% or more of the trials) and "Have Models" group (participants who aligned the model to the target diagram on less than 50% of trials)], the Use Models group ($n = 13$) was significantly more accurate ($d = 1.69$) on the diagram translation task than both the Have Models group ($n = 19$) and the No Models group ($d = 1.52$) with the latter two groups not differing statistically from one another (see Figure 2). Thus, just seeing the 3-D spatial arrangement of substituents, which is represented transparently by the models, did not offer any benefit to performance.

In addition, as in Study 1, translation accuracy was positively correlated with spatial ability. Interestingly, in this study, there was no independent contribution of spatial ability to predicting translation accuracy, after controlling for use of a model to enact the translation (i.e., aligning the model to the diagram to be drawn).

Model use was more common in Study 2 than in Study 1. In these first two studies, the models were the same rotamer as the given diagram but were presented to participants in an orientation that was not aligned with the given diagram. Without aligning the model to the given diagram, students may not have been able to see the correspondence between the two representations,[37,38] and this may have inhibited model use. The purpose of Study 3 was to test the benefit of models when participants were actively encouraged to use them, when the models were placed in their hands, and when the models were presented in the orientation corresponding to the given diagrams. The prediction was that availability of a model
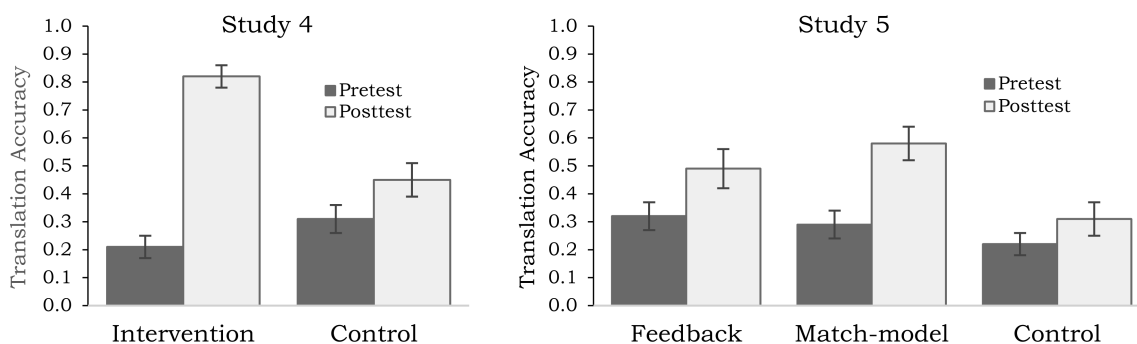
Figure 3. Means for pretest and posttest translation accuracy for the first (left) and second (right) study from Padalkar and Hegarty.[6] Translation accuracy is reported as proportion correct on diagram translations. Error bars show standard error of the mean.

would be positively associated with drawing accuracy, but only if students rotated the model to the orientation of the diagram they were required to draw (Align-Target), as in Study 2.

To test these predictions, the students were again assigned to a Models ($n = 30$) or a Control group ($n = 29$). Results indicated that although the Models group was more accurate than the Control group, the difference between the groups was not statistically significant. However, when the Models group was divided into those who used the models (Use Models group; $n = 18$) and those who had models available but did not use them (Have Models group; $n = 12$), as in Study 2, Models users were again significantly more accurate than Have Models ($d = 1.51$) and No Models groups ($d = 0.84$) (see Figure 2). As in Study 2, accuracy of the Have Models group and No Models group was not significantly different.

Similar to Studies 1 and 2, translation accuracy was again positively correlated with spatial ability. However, as in Study 2, spatial ability was not an independent predictor of translation accuracy after controlling for model use.

Stull et al.[9] concluded that models are useful when they are used by students to off-load or augment difficult mental processes. In contrast, just seeing a model of the molecule in question is not sufficient to help students perform the translation. Although spatial ability predicted performance, model use was a better predictor and in Studies 2 and 3, spatial ability was not a significant predictor after controlling for model use. These results suggest that using models when reasoning about structural diagrams is a promising way to help students develop representational competence and that using models can mitigate effects of spatial ability.

Guided Use of Models

A more vexing result from the studies of Stull et al.[9] was that many students did not use the model even when they were encouraged to do so. This could be because some students are overconfident in their ability to mentally perform spatial inference tasks without the use of models. Research in cognitive and social psychology has revealed that people are not always good at evaluating their own ability or competence[39] and can be subject to illusions of understanding, in which they believe that they understand material better than they actually do.[40−42] Specifically, students might not realize the importance of preserving 3-D relationship between the substituents when translating between different diagrams. Another possible reason for ignoring models is that students might not be able to discover the model-based strategy on their own, possibly because the use of models to make spatial inferences is difficult. To use a model in the diagram translation task, a student must

understand the correspondence between the model and the molecule it represents and that transformations of the model reveal something about the molecule.[28] However, students who do not spontaneously discover an effective strategy can often be taught the strategy.[39] Moreover, students will adopt better learning strategies, provided that they experience the benefits of the strategy.[43,44]

To address these possibilities, Padalkar and Hegarty[6] developed an intervention that provided students with model-based feedback on their performance, thereby exposing students to their illusions of understanding or competence and allowing them to experience benefits of using models. In this intervention, participants' first attempt to solve diagram translation problems in a pretest with models available. Next, they receive a model of the given diagram and have to try to rotate and reconfigure it to match the diagram they have drawn, which is only possible if they have drawn the diagram correctly. In their first study, Padalkar and Hegarty tested the effectiveness of this intervention against a control group (Study 4). In their second study, the effectiveness of each of two main components of the intervention, namely, verbal feedback on performance and active use of the models, were tested separately and compared to a control group (Study 5). Both studies followed a pretest−posttest design and used the same diagram translation tasks as Stull et al.,[8] with 6 pretest and 12 posttest problems.

Results showed that the intervention was very effective. The Intervention group ($n = 30$) used models on most problems (87% on average) after the intervention and this group showed large improvements on the posttest ($d = 2.08$) compared with the Control group ($n = 24$), as shown in Figure 3. Specifically, the intervention group was 82% correct, on average, on the posttest. Use of the models to verify translations improved students' representational competence as evidenced by the increases in performance from the pretest to the posttest. In addition, these improvements in accuracy were accompanied by improvements in student attitude toward using models in the future.

Two contributions of the intervention might explain the benefit of students using models to verify their translations. First, direct physical rotation of the models to generate feedback on their own drawings might support reasoning by enabling students to experience the benefit of models. Second, feedback received by using the model to check one's answer might address overconfidence or illusions of understanding. Study 5 was conducted to gauge the contribution of each of these two aspects of the intervention, namely, the opportunity to (1) handle and align models to diagrams and (2) receive

Table 1. Summary of Feedback Type of Test for Study 6 and 7 on the Effect of Model Use on Chemistry Learning

| Feedback Type	Pretest	Intervention	Models Posttest (same day)	No-model Posttest (same day)	Delayed Posttest (7-day delay)
Hand-held	No models	Hand-held models with verbal feedback	Hand-held models	No models	No models
Virtual	No models	Virtual models with verbal feedback	Virtual models	No models	No models
Control	No models	Verbal feedback only	No models	No models	No models
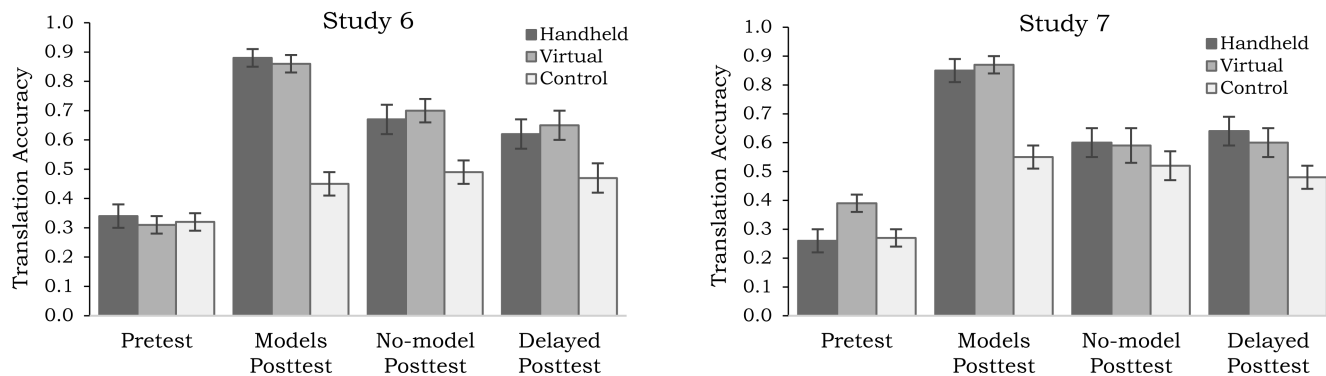
Figure 4. Mean translation accuracy for those receiving hand-held or virtual model interventions and a control group over measures of pretest and posttest performance for the first (left) and second (right) study from Stull and Hegarty.[8] Translation accuracy is reported as proportion correct on diagram translations. Error bars show standard error of the mean.

verbal feedback. The study design used three conditions. One group of participants practiced aligning models to diagrams but did not receive feedback on their pretest drawings (Match-Model group) (n = 25). A second group received verbal feedback on their solutions but did not align models to diagrams (Feedback group) (n = 25). A third group did not align models and did not receive verbal feedback (Control group) (n = 25).

As shown in Figure 3, the Match-Model group improved the most in this study, and only this group significantly outperformed the Control group on the posttest. These results suggest that failure on this task is not merely due to overconfidence or lack of understanding about the relevance of the 3-D structure. If this were true, then the verbal feedback should have been sufficient to improve performance. Rather, the results suggest that students need to experience the benefits of manipulating models, as they did in the Match-Model condition, in order to discover the model-based strategy for diagram translation. Finally, although the Match-Model group performed best on the posttest in this experiment, this group was not as successful as the intervention group in Padalkar and Hegarty's[6] first study (Study 4), suggesting that using models to receive feedback (*Model-Based Feedback*) is a particularly effective intervention.

Benefit to Long-Term Learning

The results of these previous studies clearly show that models can be useful in helping students reason about structural diagrams and that model-based feedback can increase model-use and improve problem-solving performance. These results are consistent with the idea that a molecular model serves as a cognitive scaffold[45] in the development of representational competence. Models may serve as cognitive scaffolds because they support better integration of spatial concepts by offering alternate representations of molecules, easing the demands on a student's spatial working memory by representing 3-D spatial relations directly, and supporting physical enactment of the imagined processes to improve storage in and recall from memory. However, it is also possible that when students use

models in representation translation, the model becomes a crutch rather than a scaffold to learning. This is, students may not store the information provided by the model into long-term memory so that they become dependent on models and performance is hampered when models are no longer available.

Stull and Hegarty[7] investigated whether models serve as a scaffold or a crutch. They also compared the effectiveness of hand-held and virtual models for learning. With new technologies, virtual molecular models are increasingly available (e.g., Chem 3D, Spartan, and ChemBioDraw), and it is often assumed that virtual resources are as good as, if not better than, traditional resources.[46] However, to date, research on the relative effectiveness of hand-held and virtual models is sparse in chemistry,[47−49] and there may be disadvantages to using virtual models. For example, skills learned when working with virtual models many not necessarily transfer to working with real-world objects[50] and virtual models often require more costly and elaborate equipment.

When one interacts with a hand-held model, one can sense the 3-D shape of the model through both vision and touch, one's hands are colocated with the model, and the movements that one makes with one's hands to manipulate the model are congruent with what one sees. In contrast, virtual models differ in their *action-congruence*, that is, correspondence between the actions performed with the interface and the resulting movement of the virtual model.[51,52] An example of high congruence is rotating an input device in three dimensions to see the corresponding 3-D rotation of the on-screen object; an example of low congruence is pressing a key on a keyboard to produce the same rotation—the latter is currently more common in typical chemistry classrooms. Research in human-computer interaction has indicated that mismatches between vision and haptic cues impede interaction with virtual models[50,53,54] and the added cognitive effort required when the shape, action, and location of the interface is incongruent with the viewed object may negatively affect learning with virtual models,[55] especially for low-knowledge learners.[56]

To investigate these questions, Stull and Hegarty[7] conducted two studies that compared diagram translation performance after receiving a model-based feedback intervention. Students first solved pretest problems with models and then received feedback on their answers by attempting to match models to their solutions and then solved three sets of posttest problems. In different conditions of the experiment, the feedback included matching their solution to a hand-held model (as in the intervention studied by Padalkar and Hegarty) (Study 6, n = 36; Study 7, n = 34), a virtual model (Study 6, n = 31; Study 7, n = 33), or no models (Study 6, n = 38; Study 7, n = 37). In the first posttest (Model Posttest), students in the two model groups, but not the control group, were allowed to use models. In the second posttest (No-Model Posttest), models were not available to any of the groups. Students returned 7 days later to complete the third posttest (Delayed Posttest), again without models. Table 1 summarizes the various tests and intervention conditions.

In Study 6, virtual models were manipulated with a mouse and keyboard interface, typical of commercially available virtual molecular models (low action congruence). In Study 7, virtual models were manipulated with a higher-congruence, direct manipulation interface.[49] The direct manipulation interface used a hand-held, 3-degrees-of-freedom motion tracker and stereovision glasses to minimize differences between actions performed on the interface (e.g., rotations) and the results of these actions (rotations of the model) yielding high action congruence.

Results of the studies demonstrated three important findings (see Figure 4). First, model-based feedback not only improved performance when models were available (Study 6, d = 1.81; Study 7, d = 1.39), replicating Padalkar and Hegarty,[6] but some of the benefits of models persisted when students had to solve the problems without models available. This is evident in higher performance in the No-Model Posttest for students in Study 6 (d = 0.72) who were previously trained with, but no longer had, models. Although suggestive of the same trend, no significant difference between the model groups and the control group was observed for Study 7. Second, the learning benefits achieved from the model-based intervention were resilient over a delay of 7 days. This is evident in the higher performance in the Delayed Posttest for students who received model-based training in both Study 6 (d = 0.54) and 7 (d = 0.49). Third, the format (hand-held or virtual) of the model does not appreciably affect the benefits of model-based feedback. Moreover, the virtual models with low action congruence in Study 6 were as least as effective as the virtual models with high action congruence in Study 7.

CONCLUSIONS AND RECOMMENDATIONS

This research program investigated the development of representational competence in organic chemistry by using traditional hand-held as well as virtual 3-D molecular models to help students learn to translate between multiple 2-D diagram formats. The results across seven experiments[6−8] are consistent in demonstrating that students are more successful in translating between diagrams when they have models available, that using a model to enact the translation process in the world is predictive of learning, and that a model-based feedback intervention dramatically improves learning. In addition, our work demonstrates that model-based feedback is superior to verbal feedback alone, models scaffold learning rather than act as a crutch, learning with model-based instruction is resilient

over a delay of several days, and learning with models transfers to performance when models are no longer available. Finally, our results show that hand-held models are equivalent to virtual models in promoting learning and that the level of action-congruence of the interface to the virtual model does not affect learning.

Recommendations for Chemistry Instructors

This study highlights the importance of incorporating molecular models into instruction. However, as our work demonstrates, it is not sufficient to just encourage students to purchase and use models. Instructors need to actively demonstrate how to use models in solving problems and create lecture, laboratory, and homework activities that require students to use models to reason about chemical concepts and, therefore, enable students to experience the benefits of models. It is not until students understand the value of models that they will begin to use them on their own.

Second, although it might be possible for some students to imagine the 3-D structure of molecules from diagrams and mentally transform these images, many will initially find this difficult if not impossible without the aid of models. It is well documented in the STEM literature that students with poor spatial reasoning abilities experience greater cognitive load than those with good spatial abilities because their spatial working memory capacity is more limited.[21] Our studies contribute to a body of work suggesting that the spatial reasoning skills of even low-spatial students can be developed.[57−59] This can be done by providing activities that require students to map the 3-D space directly perceived from models onto the space of 2-D diagrams, and vice versa. Specifically, to support students as they integrate the multiple representations of a molecular concept, our research suggests that models be used to enact spatial transformations and translations

Third, using models as feedback is a particularly effective way of inducing students to engage with models and experience their benefits. We encourage instructors to develop model-based activities that have students use models to check and validate prior work. In this way, students experience the benefit of models, confront any illusions of understanding or overconfidence in their performance, and can develop rich internal models so that their need to use external models can gradually fade.

Finally, our research suggests that it does not matter whether models are virtual or hand-held or employ a high- or low-congruence interface as long as students interact with and receive feedback from the models, providing new evidence for the potential of virtual resources in education. We encourage instructors to explore the wealth of computer-based visualizations that can be demonstrated in class and that can be assigned as an active component of homework.

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Notes
The authors declare no competing financial interest.

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